Generative artificial intelligence empowers digital twins in drug discovery and clinical trials

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Abstract

ABSTRACT Introduction The concept of Digital Twins (DTs) translated to drug development and clinical trials describes virtual representations of systems of various complexities, ranging from individual cells to entire humans, and enables in silico simulations and experiments. DTs increase the efficiency of drug discovery and development by digitalizing processes associated with high economic, ethical, or social burden. The impact is multifaceted: DT models sharpen disease understanding, support biomarker discovery and accelerate drug development, thus advancing precision medicine. One way to realize DTs is by generative artificial intelligence (AI), a cutting-edge technology that enables the creation of novel, realistic and complex data with desired properties. Areas covered The authors provide a brief introduction to generative AI and describe how it facilitates the modeling of DTs. In addition, they compare existing implementations of generative AI for DTs in drug discovery and clinical trials. Finally, they discuss technical and regulatory challenges that should be addressed before DTs can transform drug discovery and clinical trials. Expert opinion The current state of DTs in drug discovery and clinical trials does not exploit the entire power of generative AI yet and is limited to simulation of a small number of characteristics. Nonetheless, generative AI has the potential to transform the field by leveraging recent developments in deep learning and customizing models for the needs of scientists, physicians and patients.